## Nitrogen pumpout calc

We ask how much nitrogen is present, and how long to pump out. Assume a light tube of PMMA that is saturated with N2 at 1 atm to start. We then pull a good vacuum on it at t=0, and compute the diffusion out through the surfaces

Solubility: again from NIST reference:

**Experimental Data** Henry's law solubility constants S for gases in PMMA

Gas	Pressure/atm	$S/(cm^3(STP)/g atm)$
Не	3.8–7.2	0.066
Ne	2.7	0.126
Ar	3.2-7.4	$0.105 \pm 0.063$
Kr	2.6-4.6	0.122
$N_2$	5.7-15.0	$0.045 \pm 0.028$
CO <sub>2</sub>	4.0-19.0	$0.260 \pm 0.024$

$$S_{\text{N2\_PMMA}} \coloneqq .045 \frac{\text{scc}}{\text{gm} \cdot \text{atm}} \qquad M_{\text{a\_N2}} \coloneqq 28 \frac{\text{gm}}{\text{mol}} \qquad \text{scc} = 4.464 \times 10^{-5} \, \text{mol}$$

Light tube dims:

 $t_{lt} := 3 \text{mm}$   $l_{lt} := 1.3 \text{m}$   $r_{lt} := 53 \text{cm}$ buffer support and SiPM plane are not included here Light tube area, volume, mass:

$$A_{lt} := 4\pi r_{lt} \cdot l_{lt}$$
  $V_{lt} := 2\pi r_{lt} \cdot l_{lt} \cdot t_{lt}$   $M_{lt} := V_{lt} \cdot \rho_{PMMA}$   
 $A_{lt} = 8.658 \,\text{m}^2$   $V_{lt} = 0.013 \,\text{m}^3$   $M_{lt} = 15.585 \,\text{kg}$ 

Mass, number of moles N2

$$\begin{split} \mathbf{M}_{N2\_lt} \coloneqq \mathbf{S}_{N2\_PMMA} \mathbf{M}_{lt} \cdot \mathbf{1} \\ \mathbf{atm} \cdot \mathbf{M}_{a\_N2} & \mathbf{M}_{N2\_lt} = 0.877 \, \text{gm} & \text{(note purifier has 30 gm removal capacity, below)} \\ \mathbf{N}_{N2\_lt} \coloneqq \mathbf{S}_{N2\_PMMA} \cdot \mathbf{M}_{lt} \cdot \mathbf{1} \\ \mathbf{atm} & \mathbf{N}_{N2\_lt} = 0.031 \, \text{mol} & \mathbf{S}_m \coloneqq \frac{\mathbf{M}_{N2\_lt}}{\mathbf{M}_{lt}} & \mathbf{S}_m = 5.625 \times 10^{-5} \\ \mathbf{M}_{lt} & \mathbf{$$

Molar concentration, initial

$$C_{i\_N2} := S_{N2\_PMMA} \cdot \rho_{PMMA} \cdot 1 \text{ atm}$$
  $C_{i\_N2} = 2.411 \frac{\text{mol}}{\text{m}^3}$ 

Diffusion constant for N2 in polymers

$$D_{N2\_PMMA} := 5 \cdot 10^{-9} \frac{m^2}{s}$$
 from: -->

Solubilities and diffusion coefficients of carbon dioxide and nitrogen in polypropylene, high-density polyethylene, and polystyrene under high pressures and temperatures H.Masuoka, et al.)

## Finite thickness plane (1D) Fick's 2nd law solution:

diffusion constant:

$$D := D_{N2PMMA}$$

for plate of half thickness h, and distance from plate centerplane x, and some time after initial vacuum aplication

$$\begin{array}{ll} h:=0.5t_{1t} & x:=h & h=1.5\,\text{mm} \\ \\ \text{time unit} \\ u:=1\,\text{min} \\ \\ \text{range variable} \end{array}$$

For an infinite sheet of width 2l, with initial concentration C<sub>i</sub> suddently exposed to a surface concentration of C<sub>i</sub>, total (integrated) mass flow through surface at time t divided by the total for t = infinity:

$$1 := h$$
  $1 = 1.5 \, \text{mm}$ 

t := 1u, 2u ... 100u

$$f_{\mathbf{M}}(t) := 1 - \sum_{n=0}^{\infty} \left[ \frac{8}{(2n+1)^{2} \pi^{2}} e^{\left[ \frac{-D \cdot (2n+1)^{2} \pi^{2} t}{4l^{2}} \right]} \right]^{\mathbf{I}}$$

Mathematics of Diffusion, Crank, eq. 4.18

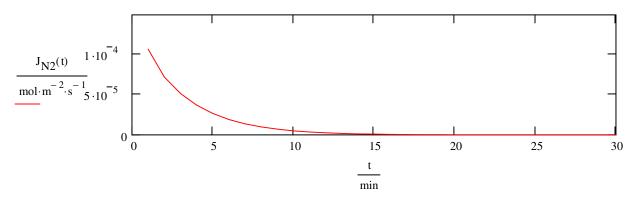
differentiating this with respect time gives us (dimensionless) flux (flow rate):

$$dfMdt(t) := \sum_{n=0}^{100} \left[ 2 \frac{D}{1^2} \cdot e^{\left[ \frac{-D \cdot (2n+1)^2 \pi^2 t}{4l^2} \right]} \right]$$

first few terms of summation are sufficient for long

and outgassing flux is then:

$$J_{N2}(t) := V_{lt} \cdot C_{i N2} \cdot dfMdt(t)$$



$$\text{check -->} \qquad \int_{0s}^{1\,day} \mathbf{J}_{N2}(t)\;dt = 0.031\,\text{mol} \label{eq:JN2}$$

initial gas load -->  $N_{N2\_lt} = 0.031 \, \text{mol}$ 

$$N_{N2}$$
 lt = 0.031 mol

95% removal time

$$t_{95} \coloneqq 8 \text{min} \qquad \int_{0s}^{t_{95}} \mathrm{J}_{N2}(t) \ \text{d}t = 0.029 \, \text{mol}$$

outgas rate after 0.1, 1 hr

$$\begin{split} t_{1hr} &:= \binom{0.1}{1} hr \\ J_{N2}(t_{1hr}) &= \binom{1.933 \times 10^{-5}}{3.723 \times 10^{-13}} \frac{mol}{s} \\ P_{1hr} &:= J_{N2}(t_{1hr}) \cdot R \cdot T \qquad P_{1hr} &= \binom{0.353}{6.802 \times 10^{-9}} \frac{torr \cdot L}{s} \end{split}$$